Studies of the Incommensurate Magnetic Structure of a Heavy Fermion System: $CeRhIn_5$

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$CeRhIn_5$ belongs to the family of heavy fermion (HF) superconductors in which superconductivity (SC) develops out of a normal state where electronic correlations produce a large enhancement of the effective mass of the conduction electrons. $CeRhIn_5$ is an antiferromagnet at ambient pressure with a Néel temperature of 3.8 K and it becomes a superconductor below $T_c = 2.1$ K when pressure is applied (1.65 GPa).

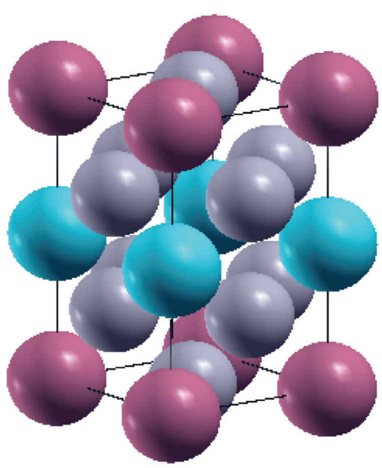

Fig. 1. ***The tetragonal crystal structure of $CeRhIn_5$. Ce, Rh, and In ions are represented by purple, cyan, and light grey balls respectively. The lattice parameters are a = 4.65 Å and c = 7.54 Å at 295 K.***

This compound crystallizes in the tetragonal $HoCoGa_5$ type of structure displayed in Fig. 1, which is also common to the ambient-pressure superconductors, $CeIrIn_5$, $CeCoIn_5$, and $PuCoGa_5$. This quasi-two-dimensional structure seems to be favorable for heavy fermion SC, in the same way as the $TlCr_2Si_2$-type is often observed in the BCS conventional superconductors as well as in some of HF superconductors. A neutron diffraction study [1] performed on $CeRhIn_5$ revealed an incommensurate magnetic structure with wave vector q = (1/2,1/2,0.297) and a staggered moment of 0.75(2) μ_B per Ce ion [2] at 1.4 K. The nearest-neighbor moments on the tetragonal basal plane align antiferromagnetically. Coexistence of antiferromagnetism (AFM) and SC under pressure (P = 1.75 GPa) in $CeRhIn_5$ has been reported [3]. Recently, neutron diffraction and electrical resistivity studies [4] determined a broader range of pressures (0.9 GPa $\leq$ P $\geq$ 1.75 GPa) than previous accounts [3], in which long-range magnetic order and SC exist simultaneously.

Our present investigation has been motivated by the interesting relation between relatively large ordered moments with unconventional SC which in $CeRhIn_5$ appears to be qualitatively different from other Ce-based HF superconductors. We performed noncollinear first principle calculations using the full-potential augmented plane-waves with local orbitals (FP-APW+lo) [5]. This method allows us to study noncollinear magnetic structures like the incommensurate structure that $CeRhIn_5$ has been reported to possesses [1]. The magnetization density is treated, in this method, as a vector field free to vary in magnitude and direction everywhere. We investigated different incommensurate structures described by the wave vector q, the ferromagnetic and the antiferromagnetic arrangement of the magnetic moments at ambient pressure. A study of the magnetic structure under pressure will be presented elsewhere.

The Ce ion possesses one 4f electron in these compounds. We used the LSDA-SIC to describe the localization of the 4f electron. We did not perform calculations with the 4f electron itinerant since previous theoretical studies and our own suggested that the f electron in this compound behaves localized. This election of the exchange correlation potential gave us consistent results regarding magnetic moments and magnetic structure.

The total energy has been plotted in Fig. 2 as function of the z-component of the wave vector q = (1/2,1/2,q_z). We have investigated the $\overline{\Gamma Z}$ line of the Brillouin zone (BZ) which runs along the z-axis. The ferromagnetic and the antiferromagnetic state are represented by q_z = 0 and q_z = 1/2 respectively. Our results (Fig. 2) show that there is a q value, that minimizes the total energy. The magnetic structure corresponds then to a spin spiral with a wavevector q_z ~ 0.2 which compares very well with the experimental value of 0.29. We are planning to study the evolution of the magnetic structure in $CeRhIn_5$ as pressure is applied, especially in the region where SC is present.

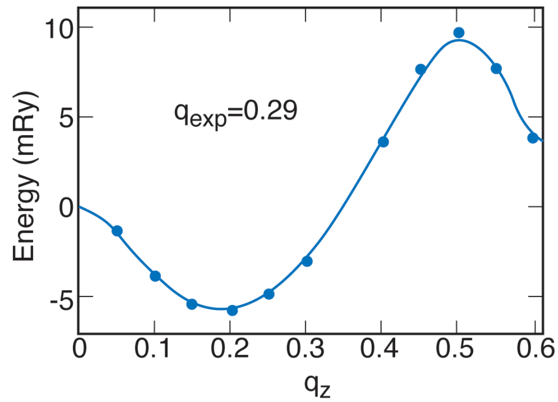

Fig. 2.
The total energy as a function of the z-component of the wave vector.

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